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DOE Office of Science Funded Basic Research at NREL that Impacts Photovoltaic Technologies

S.K. Deb

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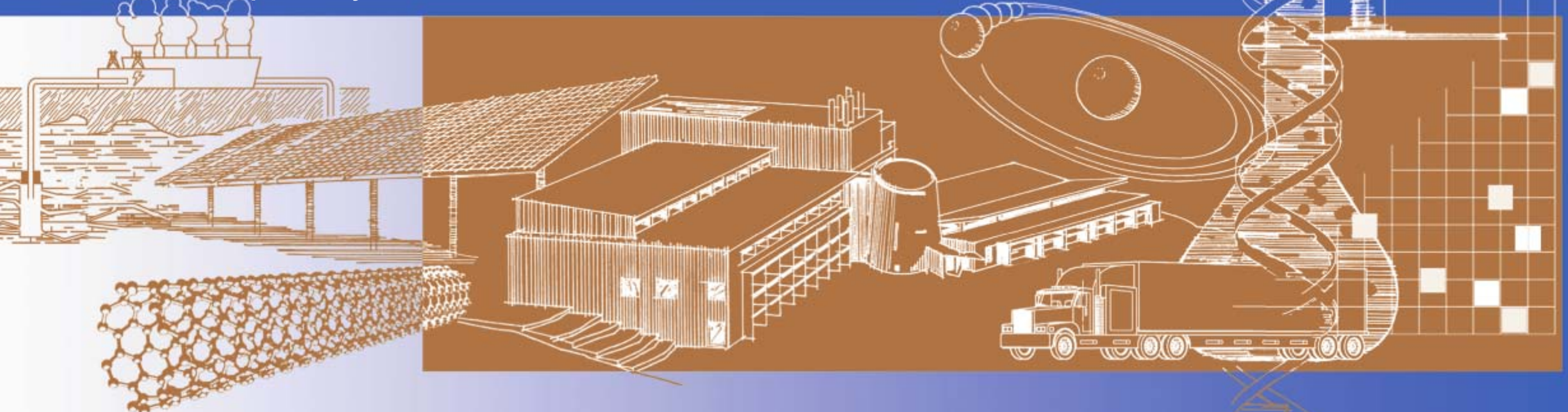

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Satyen K. Deb
National Renewable Energy Laboratory
1617 Cole Boulevard
Golden, CO 80401-3393
satyen_deb@nrel.gov

ABSTRACT

The DOE Office of Science, Basic Energy Sciences, supports a number of basic research projects in materials, chemicals, and biosciences at the National Renewable Energy Laboratory (NREL) that impact several renewable energy technologies, including photovoltaics (PV). The goal of the Material Sciences projects is to study the structural, optical, electrical, and defect properties of semiconductors and related materials using state-of-the-art experimental and theoretical techniques. Specific projects involving PV include: ordering in III-V semiconductors, isoelectronic co-doping, doping bottlenecks in semiconductors, solid-state theory, and computational science. The goal of the Chemical Sciences projects is to advance the fundamental understanding of the relevant science involving materials, photochemistry, photoelectrochemistry, nanoscale chemistry, and catalysis that support solar photochemical conversion technologies. Specific projects relating to PV include: dye-sensitized TiO_2 solar cells, semiconductor nanostructures, and molecular semiconductors. This presentation will give an overview of some of the major accomplishments of these projects.

Introduction

The DOE Office of Science, Basic Energy Sciences (BES), provides funding for a number of research projects in materials, chemicals, and biosciences at NREL that impact several renewable energy technologies, including PV. The projects funded by the Materials and Chemical Sciences primarily impact the PV technologies. The primary objective of the BES-funded project is to conduct cutting-edge fundamental research that underpins energy-related technologies. In this presentation, we will review the current status of our research activities and demonstrate how the basic research impacts PV technologies.

1. Material Sciences Projects

The goal of the material sciences project is to study the structural, optical, electrical, and defect properties of some exciting new semiconductor and related materials for PV and other energy-related technologies. Specific projects involving PV technologies include: (i) ordering of III-V semiconductor alloy materials, (ii) physics of isoelectronic co-doping, (iii) doping bottlenecks in semiconductors, (iv) solid-state theory and computational sciences, and (v) nanostructure material.

1.1 Ordering of semiconductors

The project involves experimental and theoretical studies aimed at understanding spontaneous, long-range ordering in isovalent III-V semiconductor alloys such as GaP / InP and related materials. The approaches taken involve: (i) metal-organic chemical vapor deposition / molecular-beam epitaxy (MOCVD / MBE) growth and *in-situ* characterization of III-V alloys, (ii) structural studies by transmission electron diffraction and X-ray scattering using synchrotron sources, (iii) extensive use of advanced spectroscopic techniques (such as laser Raman, photoluminescence, modulation reflectance, ellipsometry, reflectance-difference spectroscopy [RDS], and near-field scanning optical microscopy [NSOM]) for studying ordering phenomena, and (iv) theoretical studies on surface and epitaxially induced bulk ordering and its effect on electronic structures and lattice dynamics. The major impact of this work has been on developing ultra-high-efficiency (>30%) multijunction solar cells involving GaInP / GaAs / Ge. One of the key materials in these devices is GaInP, which shows CuPt ordering, which leads to changes in its electronic structure and bandgap energies. Tailoring and control of bandgap are important for device optimization.

1.2 Physics of isoelectronic co-doping of III-V semiconductors

Increasing the efficiency of multijunction ultra-high-efficiency solar cells (40%) requires the use of a novel 1-eV material that is lattice-matched to GaAs (Fig. 1). It has been shown that isoelectronic doping of GaAs and GaP with N leads to large changes in bandgap, and with N concentration of ~3%, the bandgap can be tailored to 1 eV. We are using a variety of theoretical and experimental techniques to study the role of N in optoelectronic properties of these materials. A novel extension of this work involves Bi doping and (n, Bi) co-doping of GaAs and GaP by MBE and MOCVD. A significant development in this work involves our studies on luminescence from single and isolated impurity centers, which provides an unprecedented perspective on the science of impurities at nanoscale. A novel concept has been developed of a multijunction device based on this approach that can lead to ultra-high efficiency.

1.3 Doping bottleneck in PV materials

First-principle total-energy calculations of structural and electronic properties of defects, impurities, and defect complexes in bulk and surface-related doping phenomena

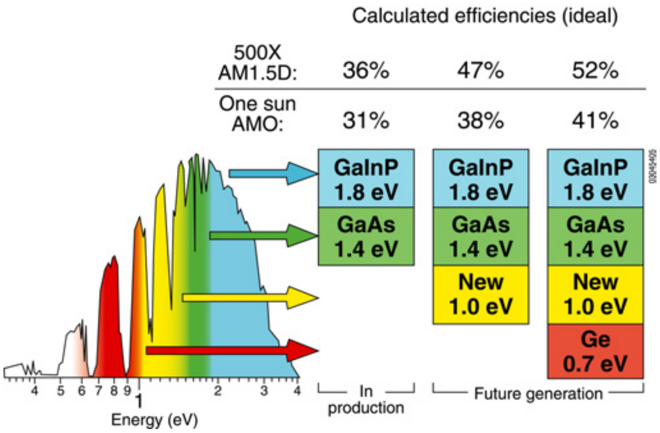

Fig. 1. A novel material with a 1-eV bandgap is instrumental in developing an ultra-high-efficiency multijunction solar cell.

enable us to understand and overcome doping limits in materials for PV applications. We established a new mechanism for doping by size-mismatched impurities in semiconductors, to achieve doping without increasing charge-compensating native defects in II-VI semiconductors.

2. Chemical Sciences Projects

The goal of the DOE / BES Chemical Sciences Program at NREL is to advance the fundamental understanding of the relevant science involving materials, photochemistry, photoelectrochemistry, nanoscale chemistry, and catalysis that support solar photochemical conversion technologies, including PV. Some of the approaches taken are (i) photoconversion using quantum dots (QDs) and QD arrays, (ii) synthesis and characterization of novel semiconductor QDs and self-organized QD structures, (iii) dye-sensitized TiO_2 solar cells, and (iv) self-organized films of liquid-crystalline molecular semiconductors and related materials for organic PV cell applications.

Dramatic variation of optical and electronic properties of semiconductor materials as a consequence of size quantization effect opens up opportunities for using nanoscale materials for developing the next generation of ultra-high-efficiency PV devices. One of the significant developments has been the demonstration of carrier multiplication by impact ionization processes in QDs and singlet fission in molecular dyes. QD solar cells hold promise for significantly enhancing efficiency of PV cells. Another area of interest is the fabrication of QD sensitized nanocrystalline TiO_2 solar cells.

NREL research on dye sensitization of TiO_2 solar cells is jointly funded by the DOE/BES Chemical Sciences Program and DOE Energy Efficiency and Renewable Energy Office (EERE) PV Program. Major progress has been made on understanding the basic physico-chemical processes in dye-sensitized solar cells.

We are also investigating doping processes in organic semiconductors for organic solar cells and studying the generation and recombination of excitons and conjugated polymer heterojunction. A fundamental understanding of optical and transport properties of molecular semiconductors impacts the design of efficient organic PV cells.

3. Conclusions

The cutting-edge research conducted at NREL provides a crucial scientific base that underpins renewable energy technologies. Synergism between BES-supported basic research and the energy technology programs supported by EERE, as well as the co-location of programs at NREL, have led to outstanding successes in the development and transfer of technology to industry. Our outstanding record of scientific accomplishments through research supported by BES and EERE has made NREL the premier research institution in the world in the field of renewable energy.

ACKNOWLEDGEMENTS

The accomplishments presented here are due largely to contributions of many of my colleagues at NREL and their collaborators. I would like to thank the program managers at DOE/BES Divisions of Materials and Chemical Sciences for their support of NREL's research effort in these areas under Contract #DE-AC-36-99-GO1033.

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